Optimizing the Hartree-Fock orbitals by the DMRG

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In this presentation, we will introduce a novel approach to optimize the Hartree-Fock orbitals by using the density matrix renormalization group. It allows, for the first time, a substantially large basis set to be accurately and efficiently optimized from 172 or more Hartree-Fock orbitals[1]. This has improved greatly the accuracy of results and is a significant advance towards the large scale application of density matrix renormalization group or other numerical methods in quantum many-body calculations. As an example, we calculated the electronic structure of a water molecule. By using just 60 optimized orbitals, we find that our result of the ground state energy of water molecule has already been beyond the accuracy of the best quantum Monte Carlo result obtained with 92 obitals. This result can be used as a reference for future study of the ground state energy of water molecule.

References

[1] H.-G. Luo, M. -P. Qin and T. Xiang, Physical Review B **81**, 235129 (2010); arXiv:1002.1287 (2010).